WHAT IS CLAIMED IS:

1. A method for generating coordinates for products in a combinatorial library based on features of corresponding building blocks, wherein distances between the coordinates represent relationships between the products, the method comprising the steps of:

(1) obtaining mapping coordinates for a subset of products in the combinatorial library;

(2) obtaining building block features for the subset of products in the combinatorial library;

(3) using a supervised machine learning approach to infer a mapping function f that transforms the building block features for each product in the subset of products to the corresponding mapping coordinates for each product in the subset of products; and

(4) encoding the mapping function f in a computer readable medium, whereby the mapping function f is useful for generating coordinates for additional products in the combinatorial library from building block features associated with the additional products.

2. The method according to claim 1, further comprising the step of:

(5) providing building blocks features for at least one additional product to the mapping function f, wherein the mapping function f outputs generated mapping coordinates for the additional product.

3. The method according to claim 1, wherein step (1) comprises generating the mapping coordinates for the subset of products.

4. The method according to claim 3, wherein step (1) further comprises the steps of:

(a) generating an initial set of mapping coordinates for the subset of products;

(b) selecting two products from the subset of products;

(c) refining the mapping coordinates of at least one product selected in step (1)(b) based on the coordinates of the two products and a distance between the two products so that the distance between the refined coordinates of the two products is more representative of the relationship between the products; and

(d) repeating steps (1)(b) and (1)(c) for additional products until a stop criterion is obtained.

5. The method according to claim 1, wherein step (1) comprises calculating the mapping coordinates for the subset of products using a dimensionality reduction algorithm.

6. The method according to claim 1, wherein step (1) comprises retrieving the mapping coordinates for the subset of products from a computer readable medium.

7. The method according to claim 1, wherein step (2) comprises the step of:

using a laboratory measured value as a feature for each building block in at least one variation site in the combinatorial library.

8. The method according to claim 1, wherein step (2) comprises the step of:

using a computed value as a feature for each building block in at least one variation site in the combinatorial library.

9. The method according to claim 1, wherein at least some of the building block features represent reagents used to construct the combinatorial library.

10. The method according to claim 1, wherein at least some of the building block features represent fragments of reagents used to construct the combinatorial library.

11. The method according to claim 1, wherein at least some of the building block features represent modified fragments of reagents used to construct the combinatorial library.

12. The method according to claim 1, wherein the mapping function *f* is encoded as a neural network.

13. The method according to claim 1, wherein the mapping function *f* is a set of specialized mapping functions f_1 through f_n, each encoded as a neural network.

14. A system for generating coordinates for products in a combinatorial library based on features of corresponding building blocks, wherein distances between the coordinates represent similarity/dissimilarity of the products, comprising:

means for obtaining mapping coordinates for a subset of products in the combinatorial library;

means for obtaining building block features for the subset of products in the combinatorial library;

means for using a supervised machine learning approach to infer a mapping function *f* that transforms the building block features for each product in the subset of products to the corresponding mapping coordinates for each product in the subset of products; and

means for encoding the mapping function *f* in a computer readable medium, whereby the mapping function *f* is useful for generating coordinates for additional products in the combinatorial library from building block features associated with the additional products.

15. The system of claim 14, further comprising:

means for providing building blocks features for at least one additional product to the mapping function *f*, wherein the mapping function *f* outputs generated mapping coordinates for the additional product.

16. The system of claim 14, wherein said means for obtaining mapping coordinates comprises:

means for generating an initial set of mapping coordinates for the subset of products;

means for selecting two products from the subset of products;

means for refining the mapping coordinates of at least one product selected based on the coordinates of the two products and a distance between the two products so that the distance between the refined coordinates of the two products is more representative of the relationship between the products; and

means for continuously selecting two products at a time and refining the mapping coordinates of at least one product selected until a stop criterion is obtained.

17. The system of claim 14, wherein a laboratory measured value is used as a feature for each building block in at least one variation site in the combinatorial library.

18. The system of claim 14, wherein a computed value is used as a feature for each building block in at least one variation site in the combinatorial library.

19. The system of claim 14, wherein at least some of the building block features represent reagents used to construct the combinatorial library.

20. The system of claim 14, wherein at least some of the building block features represent fragments of reagents used to construct the combinatorial library.

21. The system of claim 14, wherein at least some of the building block features represent modified fragments of reagents used to construct the combinatorial library.

22. The system of claim 14, wherein the mapping function f is encoded as a neural network.

23. The system of claim 14, wherein the mapping function f is a set of specialized mapping functions f_1 through f_n, each encoded as a neural network.

24. A computer program product for generating coordinates for products in a combinatorial library based on features of corresponding building blocks, wherein distances between the coordinates represent similarity/dissimilarity of the products, said computer program product comprising a computer useable medium having computer program logic recorded thereon for controlling a processor, said computer program logic comprising:

a procedure that enables said processor to obtain mapping coordinates for a subset of products in the combinatorial library;

a procedure that enables said processor to obtain building block features for the subset of products in the combinatorial library;

a procedure that enables said processor to use a supervised machine learning approach to infer a mapping function f that transforms the building block features for each product in the subset of products to the corresponding mapping coordinates for each product in the subset of products; and

a procedure that enables said processor to encode the mapping function f in a computer readable medium, whereby the mapping function f is useful for generating coordinates for additional products in the combinatorial library from building block features associated with the additional products.

25. The computer program product of claim 24, further comprising:

a procedure that enables said processor to provide building blocks features for at least one additional product to the mapping function f, wherein the mapping function f outputs generated mapping coordinates for the additional product.

26. The computer program product of claim 24, wherein said procedure that enables said processor to obtain mapping coordinates comprises:

a procedure that enables said processor to generate an initial set of mapping coordinates for the subset of products;

a procedure that enables said processor to select two products from the subset of products;

a procedure that enables said processor to refine the mapping coordinates of at least one product selected based on the coordinates of the two products and a distance between the two products so that the distance between the refined coordinates of the two products is more representative of the relationship between the products; and

a procedure that enables said processor to continue selecting two products at a time and refining the mapping coordinates of at least one product selected until a stop criterion is obtained.

27. The computer program product of claim 24, wherein a laboratory measured value is used as a feature for each building block in at least one variation site in the combinatorial library.

28. The computer program product of claim 24, wherein a computed value is used as a feature for each building block in at least one variation site in the combinatorial library.

29. The computer program product of claim 24, wherein at least some of the building block features represent reagents used to construct the combinatorial library.

30. The computer program product of claim 24, wherein at least some of the building block features represent fragments of reagents used to construct the combinatorial library.

31. The computer program product of claim 24, wherein at least some of the building block features represent modified fragments of reagents used to construct the combinatorial library.

32. The computer program product of claim 24, wherein the mapping function f is encoded as a neural network.

33. The computer program product of claim 24, wherein the mapping function f is a set of specialized mapping functions f_1 through f_n, each encoded as a neural network.

34. A method for analyzing a combinatorial library $\{f_{ijk},\ i = 1,2,\ldots,r;\ j = 1,2,\ldots,r_i;\ k = 1, 2, \ldots, n\}$, wherein r represents the number of variation sites in the library, r_i represents the number of building blocks at the i-th variation site, and n represents the number of descriptors used to characterize each reagent, the method comprising the steps of:

(1) computing at least one descriptor for each reagent of the combinatorial library;

(2) selecting a training subset of products $\{p_i,\ i = 1,2,\ldots,k\}$ of the combinatorial library;

(3) mapping the training subset of products onto $\Re^m$ using a nonlinear mapping algorithm ($p_i \rightarrow y_i,\ i = 1,2,\ldots,k,\ y_i \in \Re^m$);

(4) identifying, for each product p_i of the training subset of products, corresponding reagents $\{t_{ij},\ j = 1, 2, \ldots, r\}$ and concatenating their descriptors $f_{1t_{i1}}, f_{2t_{i2}}, \ldots, f_{rt_{ir}}$ into a single vector, x_i;

(5) training a combinatorial network to recognize the mapping $x_i \rightarrow y_i$ using input/output pairs of training set $T = \{(x_i, y_i),\ i = 1,2,\ldots,k\}$;

(6) identifying, after the combinatorial network is trained, for each product $\{p_z,\ z = 1, 2, \ldots w\}$ of the combinatorial library to be mapped onto $\Re^m$, corresponding reagents $\{t_j,\ j = 1, 2, \ldots, r\}$ and concatenating their descriptors, $f_{1t_1}, f_{2t_2}, \ldots, f_{rt_r}$, into a single vector, x_z; and

(7) mapping $x_z \rightarrow y_z$ using the trained combinatorial network, wherein y_z represents generated coordinates for product p_z.

35. The method of claim 34, wherein step (2) comprises:

selecting the training subset of products randomly.

36. The method of claim 1, wherein step (3) comprises:

(a) placing the selected training subset of products on an m-dimensional nonlinear map using randomly assigned coordinates;

(b) selecting a pair of the products having a similarity relationship;

(c) revising the coordinates of at least one of the selected pair of products based on the similarity relationship and the corresponding distance between the products on the nonlinear map; and

(d) repeating steps (b) and (c) for additional pairs of the products until the distances between the products on the m-dimensional nonlinear map are representative of the similarity relationships between the products.

37. The method of claim 34, further comprising the step of:

storing an output of the trained combinatorial network on a computer readable storage device.